

# Vibrational Spectroscopy of Energetic Decomposition of High Explosives

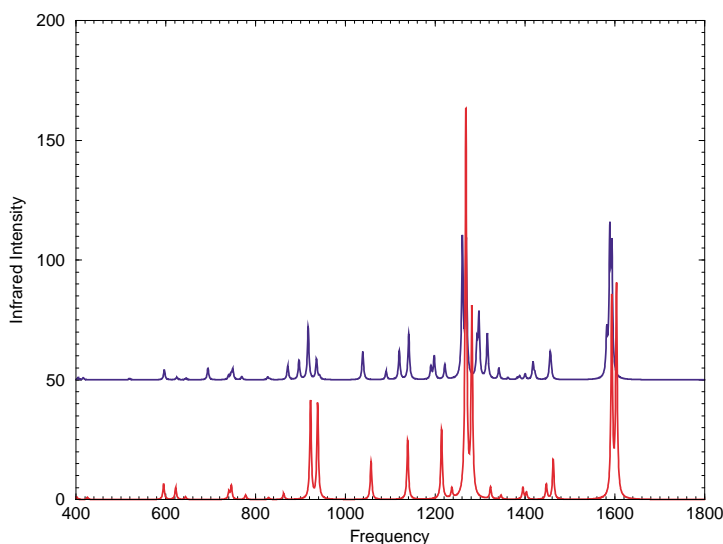
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It is experimentally observed that sudden heating of a high explosive (HE) induces changes in its vibrational spectrum that suggest breaking and rearrangement of chemical bonds amongst the atoms that form the HE molecules.

In order to ascertain the particular chemical reactions that give rise to the changes in the vibrational spectra, we make use of quantum mechanical methods to calculate the vibrational spectra of HE molecules at

various stages of decomposition and compare with the measured spectra of the heated samples. Matches and mismatches between calculated and measured spectra allow us to accept or reject possible decomposition pathways.

The Figure shows the calculated vibrational spectra of the HMX molecule before (in red) and after (in blue) loss of a  $\text{NO}_2$  group of atoms. Evidently band splitting occurs after  $\text{NO}_2$  removal.



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